



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:41 AM UTC

PDB ID : 1KBV / pdb_00001kbv
Title : NITRITE-SOAKED CRYSTAL STRUCTURE OF THE SOLUBLE DOMAIN OF ANIA FROM NEISSERIA GONORRHOEAE
Authors : Boulanger, M.J.; Murphy, M.E.P.
Deposited on : 2001-11-06
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

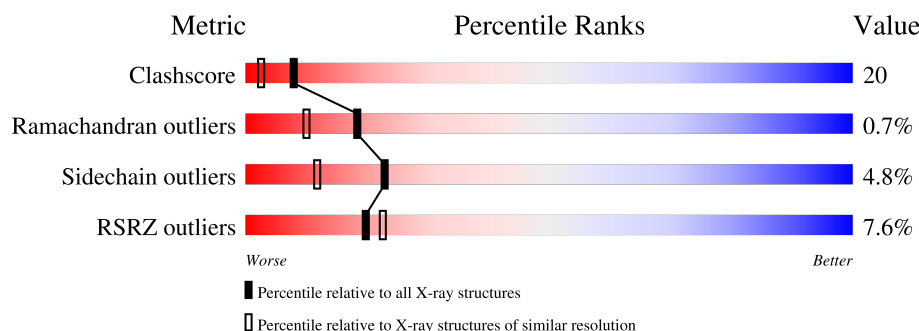
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	8% 62% 27% 8%
1	B	327	4% 60% 28% 8%
1	C	327	8% 63% 26% 8%
1	D	327	8% 61% 27% 8%
1	E	327	6% 64% 26% 8%
1	F	327	8% 60% 29% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major outer membrane protein PAN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	B	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	C	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	D	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	E	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	F	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q02219
A	209	ALA	SER	SEE REMARK 999	UNP Q02219
A	210	LEU	ILE	SEE REMARK 999	UNP Q02219
A	211	THR	ALA	SEE REMARK 999	UNP Q02219
A	283	ASN	SER	SEE REMARK 999	UNP Q02219
A	325	VAL	-	cloning artifact	UNP Q02219
A	326	PRO	-	cloning artifact	UNP Q02219
A	327	ARG	-	cloning artifact	UNP Q02219
B	1	MET	-	initiating methionine	UNP Q02219
B	209	ALA	SER	SEE REMARK 999	UNP Q02219
B	210	LEU	ILE	SEE REMARK 999	UNP Q02219
B	211	THR	ALA	SEE REMARK 999	UNP Q02219
B	283	ASN	SER	SEE REMARK 999	UNP Q02219
B	325	VAL	-	cloning artifact	UNP Q02219
B	326	PRO	-	cloning artifact	UNP Q02219
B	327	ARG	-	cloning artifact	UNP Q02219
C	1	MET	-	initiating methionine	UNP Q02219

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Chain	Residue	Modelled	Actual	Comment	Reference
C	209	ALA	SER	SEE REMARK 999	UNP Q02219
C	210	LEU	ILE	SEE REMARK 999	UNP Q02219
C	211	THR	ALA	SEE REMARK 999	UNP Q02219
C	283	ASN	SER	SEE REMARK 999	UNP Q02219
C	325	VAL	-	cloning artifact	UNP Q02219
C	326	PRO	-	cloning artifact	UNP Q02219
C	327	ARG	-	cloning artifact	UNP Q02219
D	1	MET	-	initiating methionine	UNP Q02219
D	209	ALA	SER	SEE REMARK 999	UNP Q02219
D	210	LEU	ILE	SEE REMARK 999	UNP Q02219
D	211	THR	ALA	SEE REMARK 999	UNP Q02219
D	283	ASN	SER	SEE REMARK 999	UNP Q02219
D	325	VAL	-	cloning artifact	UNP Q02219
D	326	PRO	-	cloning artifact	UNP Q02219
D	327	ARG	-	cloning artifact	UNP Q02219
E	1	MET	-	initiating methionine	UNP Q02219
E	209	ALA	SER	SEE REMARK 999	UNP Q02219
E	210	LEU	ILE	SEE REMARK 999	UNP Q02219
E	211	THR	ALA	SEE REMARK 999	UNP Q02219
E	283	ASN	SER	SEE REMARK 999	UNP Q02219
E	325	VAL	-	cloning artifact	UNP Q02219
E	326	PRO	-	cloning artifact	UNP Q02219
E	327	ARG	-	cloning artifact	UNP Q02219
F	1	MET	-	initiating methionine	UNP Q02219
F	209	ALA	SER	SEE REMARK 999	UNP Q02219
F	210	LEU	ILE	SEE REMARK 999	UNP Q02219
F	211	THR	ALA	SEE REMARK 999	UNP Q02219
F	283	ASN	SER	SEE REMARK 999	UNP Q02219
F	325	VAL	-	cloning artifact	UNP Q02219
F	326	PRO	-	cloning artifact	UNP Q02219
F	327	ARG	-	cloning artifact	UNP Q02219

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

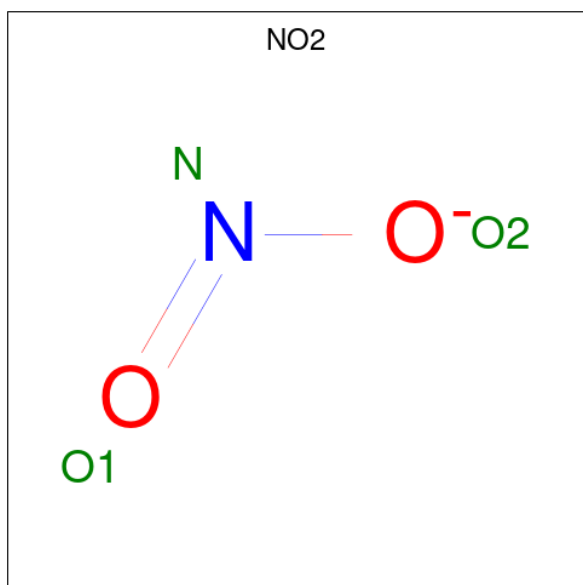
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Cu	0	0
			2	2		
2	F	2	Total	Cu	0	0
			2	2		

- Molecule 3 is NITRITE ION (CCD ID: NO2) (formula: NO₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			3	1	2		
3	A	1	Total	N	O	0	0
			3	1	2		
3	C	1	Total	N	O	0	0
			3	1	2		
3	D	1	Total	N	O	0	0
			3	1	2		
3	E	1	Total	N	O	0	0
			3	1	2		
3	F	1	Total	N	O	0	0
			3	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	377	Total	O	0	0
			377	377		

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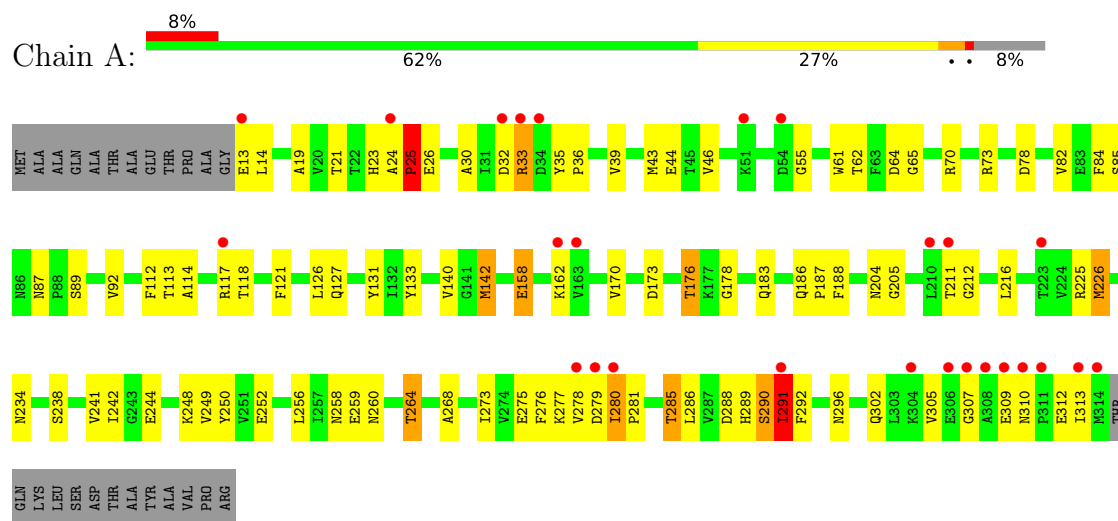
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	353	Total 353	O 353	0	0
4	C	310	Total 310	O 310	0	0
4	D	371	Total 371	O 371	0	0
4	E	317	Total 317	O 317	0	0
4	F	330	Total 330	O 330	0	0

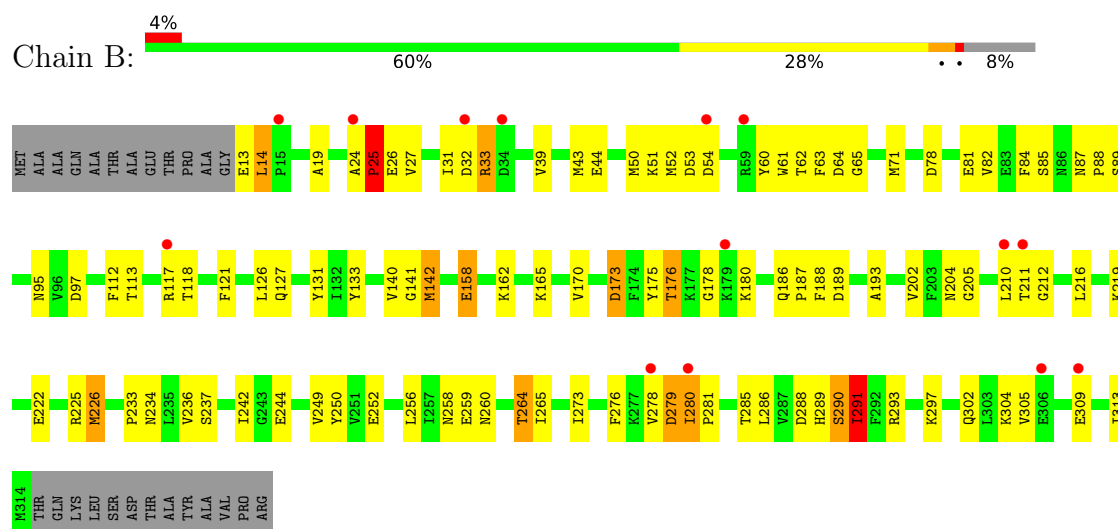
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Major outer membrane protein PAN 1

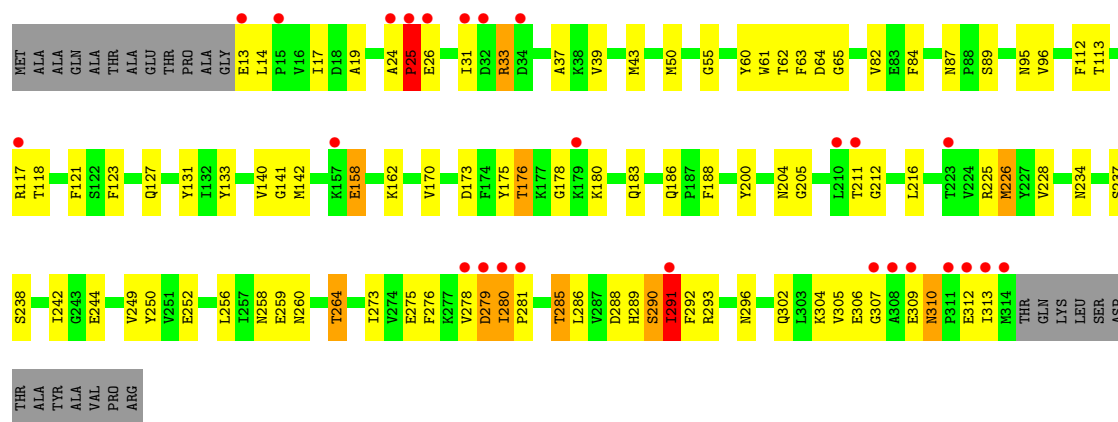


• Molecule 1: Major outer membrane protein PAN 1

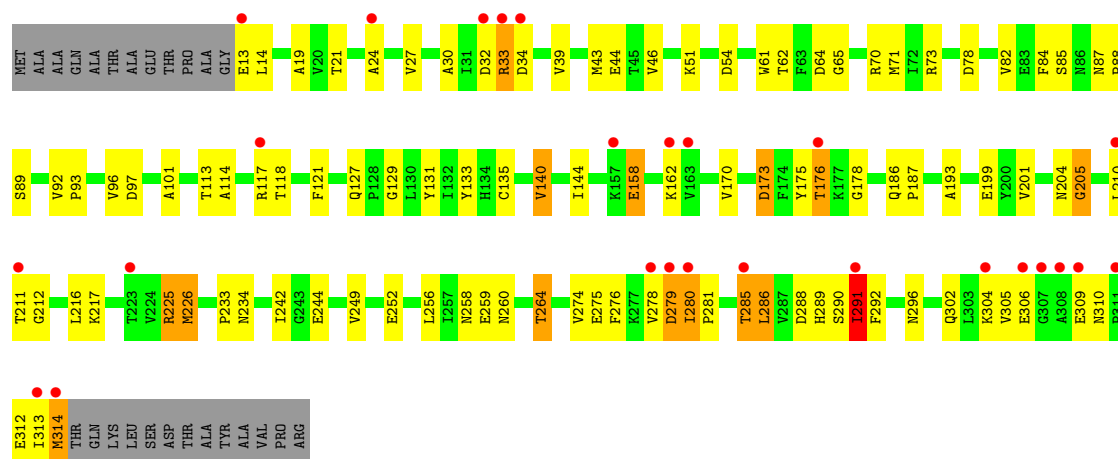


• Molecule 1: Major outer membrane protein PAN 1

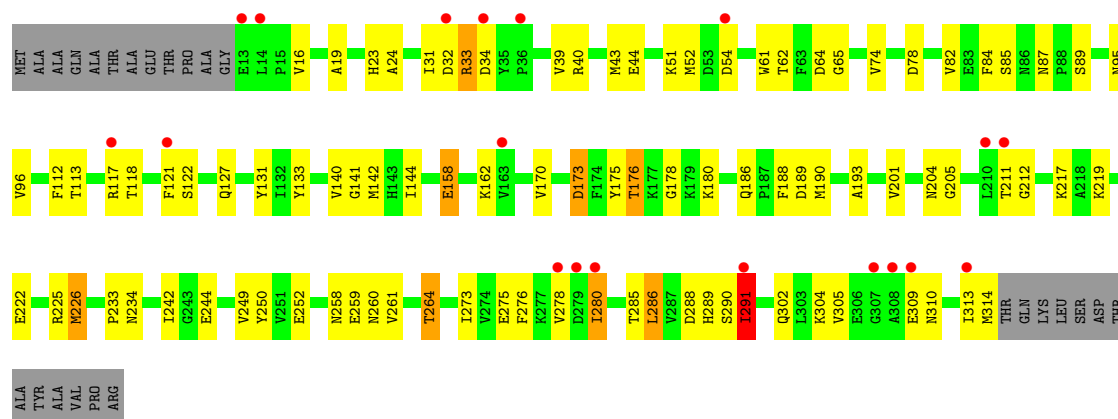




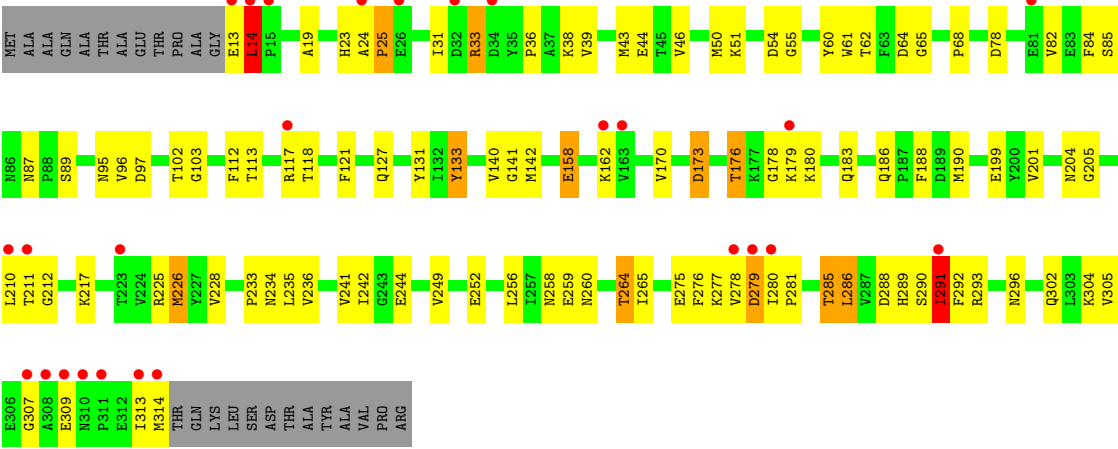
• Molecule 1: Major outer membrane protein PAN 1



• Molecule 1: Major outer membrane protein PAN 1



• Molecule 1: Major outer membrane protein PAN 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.29Å 98.09Å 102.30Å 83.89° 74.14° 73.32°	Depositor
Resolution (Å)	49.18 – 1.95 49.18 – 1.95	Depositor EDS
% Data completeness (in resolution range)	87.2 (49.18-1.95) 86.1 (49.18-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.223 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.076 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15834	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, NO2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	2/2346 (0.1%)	1.57	22/3185 (0.7%)
1	B	0.51	2/2346 (0.1%)	1.57	24/3185 (0.8%)
1	C	0.50	1/2346 (0.0%)	1.56	26/3185 (0.8%)
1	D	0.49	1/2346 (0.0%)	1.25	21/3185 (0.7%)
1	E	0.48	1/2346 (0.0%)	1.16	20/3185 (0.6%)
1	F	0.53	2/2346 (0.1%)	1.66	24/3185 (0.8%)
All	All	0.50	9/14076 (0.1%)	1.47	137/19110 (0.7%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	226	MET	SD-CE	-8.93	1.57	1.79
1	B	226	MET	SD-CE	-8.23	1.58	1.79
1	F	226	MET	SD-CE	-7.97	1.59	1.79
1	F	293	ARG	C-O	7.59	1.33	1.24
1	A	226	MET	SD-CE	-7.10	1.61	1.79
1	E	226	MET	SD-CE	-7.04	1.61	1.79
1	D	226	MET	SD-CE	-6.54	1.63	1.79
1	A	142	MET	SD-CE	-5.96	1.64	1.79
1	B	142	MET	SD-CE	-5.56	1.65	1.79

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	24	ALA	CA-C-N	47.92	179.74	119.84
1	F	24	ALA	C-N-CA	47.92	179.74	119.84
1	A	24	ALA	CA-C-N	43.13	173.76	119.84
1	A	24	ALA	C-N-CA	43.13	173.76	119.84
1	B	24	ALA	CA-C-N	42.94	173.51	119.84
1	B	24	ALA	C-N-CA	42.94	173.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ALA	CA-C-N	42.32	172.74	119.84
1	C	24	ALA	C-N-CA	42.32	172.74	119.84
1	D	24	ALA	CA-C-N	19.13	172.91	127.00
1	D	24	ALA	C-N-CA	19.13	172.91	127.00
1	D	24	ALA	C-N-CD	-18.24	80.48	120.60
1	C	24	ALA	C-N-CD	-12.82	72.44	125.00
1	A	24	ALA	C-N-CD	-12.76	72.68	125.00
1	B	24	ALA	C-N-CD	-12.76	72.69	125.00
1	D	290	SER	N-CA-C	-12.50	90.87	109.62
1	F	290	SER	N-CA-C	-12.46	90.94	109.62
1	E	24	ALA	CA-C-N	12.34	156.61	127.00
1	E	24	ALA	C-N-CA	12.34	156.61	127.00
1	B	290	SER	N-CA-C	-12.30	91.17	109.62
1	E	24	ALA	C-N-CD	-12.06	94.07	120.60
1	C	290	SER	N-CA-C	-11.79	90.64	109.39
1	A	290	SER	N-CA-C	-11.71	90.77	109.39
1	F	24	ALA	C-N-CD	-11.71	76.98	125.00
1	E	290	SER	N-CA-C	-11.70	90.80	109.39
1	A	24	ALA	N-CA-C	11.63	124.60	109.83
1	C	24	ALA	N-CA-C	11.22	124.08	109.83
1	B	24	ALA	N-CA-C	11.05	123.87	109.83
1	F	24	ALA	N-CA-C	9.62	122.05	109.83
1	D	24	ALA	N-CA-C	9.45	121.83	109.83
1	A	288	ASP	N-CA-C	-9.03	94.60	108.96
1	B	288	ASP	N-CA-C	-8.98	94.69	108.96
1	C	288	ASP	N-CA-C	-8.94	94.74	108.96
1	D	288	ASP	N-CA-C	-8.44	95.54	108.96
1	E	288	ASP	N-CA-C	-8.36	95.10	108.73
1	F	234	ASN	N-CA-C	8.33	124.13	113.88
1	E	234	ASN	N-CA-C	8.25	124.03	113.88
1	F	288	ASP	N-CA-C	-7.92	95.66	108.41
1	D	234	ASN	N-CA-C	7.81	123.48	113.88
1	C	14	LEU	N-CA-C	7.76	119.55	109.93
1	B	234	ASN	N-CA-C	7.71	123.36	113.88
1	F	309	GLU	N-CA-C	7.52	120.88	110.35
1	C	25	PRO	CA-N-CD	-7.37	101.68	112.00
1	C	234	ASN	N-CA-C	7.12	122.64	113.88
1	A	25	PRO	CA-N-CD	-7.09	102.07	112.00
1	A	234	ASN	N-CA-C	7.08	122.47	113.55
1	D	309	GLU	N-CA-C	7.07	119.97	110.35
1	C	309	GLU	N-CA-C	7.05	120.19	110.24
1	E	309	GLU	N-CA-C	7.05	120.19	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	PRO	CA-N-CD	-7.00	102.19	112.00
1	B	309	GLU	N-CA-C	6.99	120.52	110.10
1	B	131	TYR	N-CA-C	6.97	120.81	109.59
1	B	14	LEU	N-CA-C	6.94	118.65	109.83
1	E	291	ILE	N-CA-C	6.82	123.53	109.34
1	C	291	ILE	N-CA-C	6.82	123.53	109.34
1	A	131	TYR	N-CA-C	6.81	120.56	109.59
1	A	291	ILE	N-CA-C	6.81	123.50	109.34
1	E	61	TRP	N-CA-C	-6.75	97.90	108.90
1	B	291	ILE	N-CA-C	6.74	123.36	109.34
1	C	131	TYR	N-CA-C	6.70	120.37	109.59
1	A	238	SER	N-CA-C	-6.68	100.29	109.71
1	F	291	ILE	N-CA-C	6.67	123.22	109.34
1	F	131	TYR	N-CA-C	6.64	120.28	109.59
1	F	25	PRO	CA-N-CD	-6.58	102.78	112.00
1	A	309	GLU	N-CA-C	6.58	119.91	110.10
1	F	205	GLY	N-CA-C	6.54	128.68	113.18
1	D	131	TYR	N-CA-C	6.54	120.11	109.59
1	C	238	SER	N-CA-C	-6.53	100.50	109.71
1	B	61	TRP	N-CA-C	-6.51	97.80	108.41
1	A	61	TRP	N-CA-C	-6.48	97.95	108.52
1	F	65	GLY	N-CA-C	6.46	122.38	114.69
1	E	205	GLY	N-CA-C	6.45	128.48	113.18
1	C	205	GLY	N-CA-C	6.41	128.38	113.18
1	B	205	GLY	N-CA-C	6.35	128.23	113.18
1	C	61	TRP	N-CA-C	-6.35	98.17	108.52
1	C	64	ASP	N-CA-C	6.35	120.37	112.24
1	F	64	ASP	N-CA-C	6.34	120.30	111.74
1	E	131	TYR	N-CA-C	6.33	119.77	109.59
1	E	62	THR	N-CA-C	6.28	119.25	109.52
1	A	64	ASP	N-CA-C	6.27	120.27	112.24
1	F	62	THR	N-CA-C	6.27	119.24	109.52
1	F	61	TRP	N-CA-C	-6.26	98.31	108.52
1	B	65	GLY	N-CA-C	6.23	123.31	115.21
1	D	61	TRP	N-CA-C	-6.23	98.25	108.41
1	D	205	GLY	N-CA-C	6.20	127.87	113.18
1	A	205	GLY	N-CA-C	6.11	127.65	113.18
1	E	64	ASP	N-CA-C	6.09	120.01	112.58
1	F	293	ARG	CA-C-O	-5.97	113.11	119.97
1	A	14	LEU	N-CA-C	5.94	119.30	110.39
1	B	64	ASP	N-CA-C	5.93	119.84	112.24
1	D	64	ASP	N-CA-C	5.89	119.78	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	THR	N-CA-C	5.83	118.56	109.52
1	A	65	GLY	N-CA-C	5.83	122.79	115.21
1	C	65	GLY	N-CA-C	5.83	122.50	114.92
1	F	293	ARG	N-CA-C	-5.77	105.13	111.82
1	E	65	GLY	N-CA-C	5.72	122.64	115.21
1	B	62	THR	N-CA-C	5.65	118.28	109.52
1	A	62	THR	N-CA-C	5.65	117.99	109.41
1	B	133	TYR	N-CA-C	-5.64	100.59	109.50
1	B	140	VAL	N-CA-C	5.59	116.23	110.36
1	D	290	SER	CA-C-N	5.56	131.98	121.97
1	D	290	SER	C-N-CA	5.56	131.98	121.97
1	C	140	VAL	N-CA-C	5.55	116.19	110.36
1	C	62	THR	N-CA-C	5.52	118.08	109.52
1	A	140	VAL	N-CA-C	5.51	116.14	110.36
1	C	133	TYR	N-CA-C	-5.51	100.80	109.50
1	E	133	TYR	N-CA-C	-5.49	100.82	109.50
1	D	65	GLY	N-CA-C	5.48	122.34	115.21
1	F	14	LEU	N-CA-C	5.48	121.92	109.81
1	D	14	LEU	N-CA-C	5.42	118.00	110.20
1	A	126	LEU	N-CA-C	5.39	118.08	111.82
1	D	140	VAL	N-CA-C	5.36	115.99	110.36
1	A	133	TYR	N-CA-C	-5.32	101.09	109.50
1	D	199	GLU	N-CA-C	-5.31	106.93	113.41
1	B	126	LEU	N-CA-C	5.30	117.97	111.82
1	F	235	LEU	N-CA-C	5.30	118.33	110.48
1	C	228	VAL	N-CA-C	5.29	115.20	107.37
1	B	52	MET	N-CA-C	-5.27	106.53	113.12
1	D	133	TYR	N-CA-C	-5.23	101.23	109.50
1	C	310	ASN	CA-C-N	5.21	124.87	119.56
1	C	310	ASN	C-N-CA	5.21	124.87	119.56
1	B	237	SER	N-CA-C	5.20	118.08	109.46
1	F	201	VAL	N-CA-C	-5.19	100.05	107.78
1	B	63	PHE	N-CA-C	-5.18	99.33	108.20
1	C	216	LEU	N-CA-C	-5.18	103.55	110.55
1	C	63	PHE	N-CA-C	-5.18	99.35	108.20
1	A	216	LEU	N-CA-C	-5.17	103.57	110.55
1	E	140	VAL	N-CA-C	5.16	115.78	110.36
1	F	228	VAL	N-CA-C	5.15	115.27	107.80
1	E	201	VAL	N-CA-C	-5.14	100.17	107.77
1	E	310	ASN	CA-C-N	5.08	124.74	119.56
1	E	310	ASN	C-N-CA	5.08	124.74	119.56
1	D	201	VAL	N-CA-C	-5.07	100.22	107.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	SER	N-CA-C	5.07	117.87	109.46
1	F	133	TYR	N-CA-C	-5.06	100.79	109.24
1	B	202	VAL	N-CA-C	5.02	115.93	108.65
1	E	52	MET	N-CA-C	-5.02	106.85	113.12
1	F	140	VAL	N-CA-C	5.01	115.62	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2291	0	2234	102	0
1	B	2291	0	2234	88	0
1	C	2291	0	2234	84	0
1	D	2291	0	2234	111	0
1	E	2291	0	2234	92	0
1	F	2291	0	2234	105	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	6	0	0	2	0
3	C	3	0	0	1	0
3	D	3	0	0	1	0
3	E	3	0	0	1	0
3	F	3	0	0	1	0
4	A	377	0	0	12	0
4	B	353	0	0	7	0
4	C	310	0	0	5	0
4	D	371	0	0	16	0
4	E	317	0	0	10	0
4	F	330	0	0	8	0
All	All	15834	0	13404	535	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (535) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:VAL:HG11	1:E:305:VAL:HG21	1.22	1.18
1:C:278:VAL:HG11	1:C:305:VAL:HG21	1.31	1.10
1:B:278:VAL:HG11	1:B:305:VAL:HG21	1.34	1.09
1:D:278:VAL:HG11	1:D:305:VAL:HG21	1.40	1.03
1:E:249:VAL:HG11	1:E:264:THR:HG21	1.42	1.01
1:F:278:VAL:HG11	1:F:305:VAL:HG21	1.38	1.01
1:B:226:MET:HE2	1:B:276:PHE:HE2	1.30	0.95
1:A:249:VAL:HG11	1:A:264:THR:HG21	1.50	0.94
1:A:278:VAL:HG11	1:A:305:VAL:HG21	1.50	0.94
1:B:249:VAL:HG11	1:B:264:THR:HG21	1.49	0.93
1:D:249:VAL:HG11	1:D:264:THR:HG21	1.52	0.92
1:B:51:LYS:HE3	4:B:675:HOH:O	1.71	0.90
1:E:144:ILE:HD13	1:F:291:ILE:CD1	2.03	0.88
1:C:43:MET:HE2	1:C:82:VAL:HG11	1.56	0.88
1:A:117:ARG:HD3	4:A:2546:HOH:O	1.72	0.87
1:F:258:ASN:HD22	1:F:259:GLU:H	1.22	0.86
1:C:249:VAL:HG11	1:C:264:THR:HG21	1.56	0.86
1:F:176:THR:HG23	1:F:186:GLN:HB3	1.57	0.86
1:F:226:MET:HE2	1:F:276:PHE:HE2	1.41	0.86
1:C:226:MET:HE2	1:C:276:PHE:HE2	1.40	0.85
1:D:252:GLU:OE1	1:E:264:THR:HG22	1.76	0.85
1:A:226:MET:HE2	1:A:276:PHE:HE2	1.41	0.84
1:E:144:ILE:CD1	1:F:291:ILE:HD13	2.08	0.83
1:F:280:ILE:HD11	1:F:313:ILE:HB	1.61	0.83
3:A:2504:NO2:N	1:B:242:ILE:HG12	1.93	0.82
1:D:226:MET:HE2	1:D:276:PHE:HE2	1.44	0.82
1:D:32:ASP:CB	4:D:2790:HOH:O	2.28	0.81
1:A:113:THR:HA	1:A:117:ARG:NH1	1.96	0.81
1:A:252:GLU:OE1	1:B:264:THR:HG22	1.80	0.80
1:B:244:GLU:HG2	1:B:276:PHE:CD1	2.17	0.80
1:E:226:MET:HE2	1:E:276:PHE:HE2	1.47	0.80
1:B:87:ASN:HD22	1:B:89:SER:H	1.28	0.80
1:E:280:ILE:HD11	1:E:313:ILE:HB	1.63	0.80
1:F:242:ILE:HG12	3:F:2508:NO2:N	1.97	0.80
1:D:176:THR:HG23	1:D:186:GLN:HB3	1.64	0.79
1:D:314:MET:HG3	1:F:103:GLY:HA3	1.63	0.79
1:B:176:THR:HG23	1:B:186:GLN:HB3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ASN:HD22	1:C:259:GLU:H	1.27	0.79
1:E:113:THR:HG23	1:E:117:ARG:HD2	1.64	0.79
1:D:117:ARG:HD3	4:D:2786:HOH:O	1.81	0.78
1:A:242:ILE:HD12	1:A:285:THR:HG23	1.65	0.78
1:A:176:THR:HG22	1:A:178:GLY:O	1.83	0.78
1:A:113:THR:HA	1:A:117:ARG:HH11	1.49	0.78
1:D:140:VAL:O	1:D:144:ILE:HD13	1.84	0.78
1:A:113:THR:HG23	1:A:117:ARG:HD2	1.66	0.78
1:F:43:MET:HE2	1:F:82:VAL:HG11	1.67	0.77
1:A:225:ARG:HG3	1:A:275:GLU:HG2	1.66	0.76
1:D:280:ILE:HD11	1:D:313:ILE:HB	1.64	0.76
1:C:117:ARG:HG2	1:C:118:THR:N	2.00	0.76
1:F:225:ARG:HG3	1:F:275:GLU:HG2	1.69	0.75
1:E:242:ILE:HG12	3:E:2507:NO2:N	2.01	0.75
1:D:51:LYS:HE3	1:D:54:ASP:HA	1.69	0.75
1:B:226:MET:HE2	1:B:276:PHE:CE2	2.20	0.75
1:C:278:VAL:HG11	1:C:305:VAL:CG2	2.13	0.75
1:A:242:ILE:HG12	3:A:2506:NO2:N	2.01	0.75
1:C:176:THR:HG23	1:C:186:GLN:HB3	1.69	0.75
1:A:87:ASN:HD22	1:A:89:SER:H	1.35	0.74
1:B:280:ILE:CD1	1:B:313:ILE:HB	2.17	0.74
1:D:70:ARG:CZ	4:D:2603:HOH:O	2.35	0.73
1:F:278:VAL:HG11	1:F:305:VAL:CG2	2.17	0.73
1:B:176:THR:HG22	1:B:178:GLY:O	1.89	0.73
1:D:43:MET:HE2	1:D:82:VAL:HG11	1.71	0.73
1:E:144:ILE:HD12	1:F:291:ILE:HD13	1.70	0.73
1:E:176:THR:HG22	1:E:178:GLY:O	1.89	0.73
1:E:280:ILE:CD1	1:E:313:ILE:HB	2.18	0.73
1:D:258:ASN:HD22	1:D:259:GLU:H	1.37	0.72
1:F:31:ILE:CG2	1:F:33:ARG:HG3	2.18	0.72
1:C:113:THR:HG23	1:C:117:ARG:HD2	1.72	0.72
1:D:176:THR:HG22	1:D:178:GLY:O	1.90	0.72
1:C:242:ILE:HG12	3:C:2505:NO2:N	2.04	0.72
1:A:32:ASP:CB	4:A:2599:HOH:O	2.38	0.71
1:D:225:ARG:HG3	1:D:275:GLU:HG2	1.73	0.71
1:A:117:ARG:HG2	1:A:118:THR:N	2.04	0.71
1:A:264:THR:HG22	1:C:252:GLU:OE1	1.91	0.71
1:C:176:THR:HG22	1:C:178:GLY:O	1.90	0.71
1:D:127:GLN:HE21	1:E:260:ASN:HD22	1.37	0.71
1:A:43:MET:HE2	1:A:82:VAL:HG11	1.73	0.70
1:E:117:ARG:HG2	1:E:118:THR:N	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASN:HD22	1:C:89:SER:H	1.37	0.70
1:B:280:ILE:HD11	1:B:313:ILE:HB	1.75	0.69
1:C:280:ILE:CD1	1:C:313:ILE:HB	2.23	0.69
1:F:117:ARG:HG2	1:F:118:THR:N	2.07	0.69
1:F:291:ILE:CD1	4:F:2526:HOH:O	2.41	0.69
1:B:117:ARG:HG2	1:B:118:THR:N	2.05	0.69
1:F:258:ASN:HD22	1:F:259:GLU:N	1.89	0.69
1:F:280:ILE:CD1	1:F:313:ILE:HB	2.22	0.69
1:E:162:LYS:HA	1:E:162:LYS:HE2	1.75	0.69
1:A:258:ASN:HD22	1:A:259:GLU:H	1.40	0.68
1:D:242:ILE:HG12	3:D:2509:NO2:N	2.07	0.68
1:A:127:GLN:HE21	1:B:260:ASN:HD22	1.41	0.68
1:F:176:THR:HG22	1:F:178:GLY:O	1.93	0.68
1:B:278:VAL:HG11	1:B:305:VAL:CG2	2.19	0.68
1:A:211:THR:HG22	1:A:212:GLY:N	2.09	0.68
1:B:280:ILE:HG13	1:B:313:ILE:HD12	1.76	0.68
1:D:13:GLU:N	4:D:2660:HOH:O	2.27	0.67
1:F:226:MET:HE2	1:F:276:PHE:CE2	2.26	0.67
1:D:211:THR:HG22	1:D:212:GLY:N	2.08	0.67
1:B:142:MET:HE2	1:B:188:PHE:CE2	2.30	0.67
1:B:162:LYS:HE2	1:B:162:LYS:HA	1.77	0.67
1:D:211:THR:HG23	1:D:302:GLN:CD	2.19	0.67
1:F:162:LYS:HE2	1:F:162:LYS:HA	1.76	0.67
1:E:144:ILE:HD13	1:F:291:ILE:HD11	1.75	0.67
1:F:13:GLU:N	4:F:2541:HOH:O	2.27	0.67
1:E:142:MET:HE2	1:E:188:PHE:CE2	2.30	0.67
1:C:43:MET:HE2	1:C:82:VAL:CG1	2.25	0.67
1:E:173:ASP:OD1	1:E:233:PRO:HD2	1.95	0.67
1:B:113:THR:HG23	1:B:117:ARG:HD2	1.78	0.66
1:D:264:THR:HG22	1:F:252:GLU:OE1	1.94	0.66
1:C:162:LYS:HA	1:C:162:LYS:HE2	1.77	0.66
1:E:19:ALA:HB2	1:E:39:VAL:CG1	2.26	0.66
1:D:278:VAL:HG11	1:D:305:VAL:CG2	2.21	0.66
1:E:176:THR:HG23	1:E:186:GLN:HB3	1.77	0.66
1:A:43:MET:HE3	1:A:84:PHE:HD1	1.61	0.66
1:E:289:HIS:C	1:E:291:ILE:N	2.53	0.66
1:A:278:VAL:HG11	1:A:305:VAL:CG2	2.25	0.66
1:E:278:VAL:HG11	1:E:305:VAL:CG2	2.14	0.65
1:F:87:ASN:HD22	1:F:89:SER:H	1.44	0.65
1:A:280:ILE:CD1	1:A:313:ILE:HB	2.26	0.65
1:B:117:ARG:HG2	1:B:118:THR:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ALA:HB2	1:B:39:VAL:CG1	2.25	0.65
1:D:280:ILE:CD1	1:D:313:ILE:HB	2.27	0.65
1:C:31:ILE:CG2	1:C:33:ARG:HG3	2.27	0.65
1:F:249:VAL:HG11	1:F:264:THR:HG21	1.79	0.64
1:A:176:THR:HG23	1:A:186:GLN:HB3	1.79	0.64
1:B:211:THR:HG22	1:B:212:GLY:N	2.11	0.64
1:C:242:ILE:HB	1:C:285:THR:HG23	1.80	0.64
1:C:117:ARG:HG2	1:C:118:THR:H	1.63	0.64
1:A:278:VAL:CG1	1:A:305:VAL:HG11	2.27	0.64
1:D:93:PRO:HD2	4:D:2852:HOH:O	1.96	0.64
1:E:258:ASN:HD22	1:E:259:GLU:H	1.45	0.64
1:F:278:VAL:CG1	1:F:305:VAL:HG11	2.27	0.64
1:C:55:GLY:HA3	1:C:183:GLN:HE22	1.62	0.64
1:D:27:VAL:HG13	1:D:71:MET:HE2	1.80	0.64
1:E:117:ARG:HG2	1:E:118:THR:H	1.62	0.63
1:A:252:GLU:OE1	1:B:264:THR:CG2	2.47	0.63
1:A:226:MET:HE2	1:A:276:PHE:CE2	2.31	0.63
1:A:242:ILE:HD12	1:A:285:THR:CG2	2.28	0.63
1:A:114:ALA:H	1:A:117:ARG:CZ	2.10	0.63
1:E:244:GLU:HG2	1:E:276:PHE:CD1	2.34	0.63
1:C:43:MET:HE3	1:C:84:PHE:HD1	1.63	0.63
1:C:258:ASN:HD22	1:C:259:GLU:N	1.96	0.63
1:E:280:ILE:HG13	1:E:313:ILE:HD12	1.80	0.63
1:C:211:THR:HG22	1:C:212:GLY:N	2.14	0.63
1:A:256:LEU:HB2	1:B:258:ASN:ND2	2.14	0.63
1:D:170:VAL:H	1:D:204:ASN:ND2	1.97	0.62
1:A:211:THR:HG23	1:A:302:GLN:CD	2.24	0.62
1:E:225:ARG:HG3	1:E:275:GLU:HG2	1.81	0.62
1:E:252:GLU:OE1	1:F:264:THR:HG23	2.00	0.62
1:D:211:THR:CG2	1:D:212:GLY:N	2.63	0.62
1:D:87:ASN:HD22	1:D:89:SER:H	1.48	0.62
1:D:217:LYS:HE2	1:D:304:LYS:HD3	1.82	0.62
1:E:211:THR:HG22	1:E:212:GLY:N	2.14	0.62
1:F:13:GLU:HG3	1:F:13:GLU:O	1.99	0.62
1:F:158:GLU:CD	1:F:158:GLU:H	2.07	0.62
1:F:19:ALA:HB2	1:F:39:VAL:HG12	1.81	0.61
1:C:289:HIS:C	1:C:291:ILE:N	2.56	0.61
1:A:43:MET:HE2	1:A:82:VAL:CG1	2.31	0.61
1:F:43:MET:HE2	1:F:82:VAL:CG1	2.30	0.61
1:F:278:VAL:HG12	1:F:305:VAL:HG11	1.82	0.61
1:F:291:ILE:HD12	4:F:2526:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LYS:HE2	1:B:53:ASP:O	2.01	0.61
1:F:242:ILE:HB	1:F:285:THR:HG23	1.82	0.60
1:D:43:MET:HE2	1:D:82:VAL:CG1	2.31	0.60
1:C:225:ARG:NH1	1:C:275:GLU:OE2	2.34	0.60
1:E:189:ASP:OD2	4:E:2566:HOH:O	2.16	0.60
1:C:278:VAL:CG1	1:C:305:VAL:HG21	2.20	0.60
1:C:280:ILE:HD11	1:C:313:ILE:HB	1.82	0.60
1:D:242:ILE:HD12	1:D:285:THR:HG23	1.82	0.60
1:C:158:GLU:H	1:C:158:GLU:CD	2.07	0.60
1:E:144:ILE:CD1	1:F:291:ILE:CD1	2.70	0.60
1:C:244:GLU:HG2	1:C:276:PHE:CD1	2.36	0.60
1:F:117:ARG:HG2	1:F:118:THR:H	1.66	0.60
1:C:226:MET:HE2	1:C:276:PHE:CE2	2.30	0.60
1:B:87:ASN:ND2	1:B:89:SER:H	1.99	0.60
1:D:19:ALA:HB2	1:D:39:VAL:CG1	2.32	0.59
1:D:170:VAL:H	1:D:204:ASN:HD21	1.50	0.59
1:D:258:ASN:ND2	1:D:259:GLU:H	2.00	0.59
1:F:43:MET:HE3	1:F:84:PHE:HD1	1.67	0.59
1:F:211:THR:HG22	1:F:212:GLY:N	2.17	0.59
1:B:280:ILE:HD12	1:B:313:ILE:HB	1.84	0.59
1:F:113:THR:HG23	1:F:117:ARG:HD2	1.84	0.59
1:A:211:THR:CG2	1:A:212:GLY:N	2.66	0.59
1:C:19:ALA:HB2	1:C:39:VAL:HG12	1.83	0.59
1:A:87:ASN:ND2	1:A:89:SER:H	2.01	0.59
1:A:13:GLU:HG3	4:A:2647:HOH:O	2.03	0.58
1:A:162:LYS:HE2	1:A:162:LYS:HA	1.85	0.58
1:A:280:ILE:HD11	1:A:313:ILE:HB	1.85	0.58
1:D:135:CYS:O	1:D:144:ILE:HD11	2.02	0.58
1:A:13:GLU:N	4:A:2618:HOH:O	2.37	0.58
1:E:87:ASN:HD22	1:E:89:SER:H	1.51	0.58
1:A:43:MET:HE3	1:A:84:PHE:CD1	2.39	0.58
1:D:158:GLU:CD	1:D:158:GLU:H	2.10	0.58
1:B:141:GLY:HA2	1:C:291:ILE:HG21	1.86	0.58
1:D:117:ARG:HG2	1:D:118:THR:N	2.17	0.57
1:F:304:LYS:NZ	1:F:304:LYS:HB3	2.19	0.57
1:D:278:VAL:CG1	1:D:305:VAL:HG11	2.34	0.57
1:F:258:ASN:ND2	1:F:259:GLU:H	1.99	0.57
1:F:242:ILE:HD12	1:F:285:THR:HG23	1.87	0.57
1:A:158:GLU:H	1:A:158:GLU:CD	2.12	0.57
1:A:256:LEU:H	1:B:258:ASN:ND2	2.02	0.57
1:D:13:GLU:HG3	4:D:2604:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:ALA:HB2	1:F:39:VAL:CG1	2.34	0.57
1:F:225:ARG:CG	1:F:275:GLU:HG2	2.34	0.57
1:D:244:GLU:HG2	1:D:276:PHE:CD1	2.40	0.56
1:D:226:MET:HE2	1:D:276:PHE:CE2	2.33	0.56
1:A:19:ALA:HB2	1:A:39:VAL:HG12	1.88	0.56
1:A:248:LYS:HE3	1:A:275:GLU:OE1	2.05	0.56
1:D:30:ALA:HA	1:D:73:ARG:CZ	2.36	0.56
1:B:158:GLU:CD	1:B:158:GLU:H	2.12	0.56
1:A:19:ALA:HB2	1:A:39:VAL:CG1	2.35	0.56
1:B:19:ALA:HB2	1:B:39:VAL:HG12	1.87	0.56
1:B:127:GLN:HE21	1:C:260:ASN:HD22	1.54	0.56
1:B:211:THR:CG2	1:B:212:GLY:N	2.68	0.56
1:E:127:GLN:HE21	1:F:260:ASN:HD22	1.53	0.56
1:D:306:GLU:HG3	4:D:2662:HOH:O	2.06	0.56
1:E:289:HIS:C	1:E:291:ILE:H	2.13	0.56
1:F:50:MET:HE3	1:F:60:TYR:CD1	2.40	0.56
1:C:43:MET:HE1	1:C:96:VAL:HG11	1.88	0.56
1:A:256:LEU:H	1:B:258:ASN:HD21	1.52	0.55
1:B:33:ARG:HH22	1:B:78:ASP:CG	2.14	0.55
1:C:278:VAL:CG1	1:C:305:VAL:HG11	2.36	0.55
1:A:241:VAL:HG22	1:A:286:LEU:HD22	1.89	0.55
1:F:278:VAL:CG1	1:F:305:VAL:HG21	2.26	0.55
1:A:278:VAL:HG12	1:A:278:VAL:O	2.06	0.55
1:A:92:VAL:HG12	4:A:2558:HOH:O	2.06	0.55
1:B:33:ARG:NH2	1:B:78:ASP:OD2	2.39	0.55
1:B:290:SER:HB2	1:B:293:ARG:HD2	1.87	0.55
1:A:33:ARG:HH22	1:A:78:ASP:CG	2.13	0.55
1:D:34:ASP:CG	4:D:2600:HOH:O	2.49	0.55
1:C:19:ALA:HB2	1:C:39:VAL:CG1	2.36	0.55
1:C:280:ILE:HD12	1:C:313:ILE:HB	1.87	0.55
1:D:278:VAL:HG12	1:D:305:VAL:HG11	1.88	0.55
1:E:43:MET:HE2	1:E:82:VAL:HG11	1.88	0.55
1:B:13:GLU:HG3	1:B:14:LEU:N	2.22	0.55
1:A:23:HIS:CE1	4:A:2538:HOH:O	2.60	0.54
1:D:87:ASN:ND2	1:D:89:SER:H	2.05	0.54
1:C:170:VAL:H	1:C:204:ASN:ND2	2.05	0.54
1:F:211:THR:HG23	1:F:302:GLN:CD	2.33	0.54
1:C:43:MET:HE3	1:C:84:PHE:CD1	2.42	0.54
1:C:211:THR:HG23	1:C:302:GLN:CD	2.33	0.54
1:D:260:ASN:HD22	1:F:127:GLN:HE21	1.56	0.54
1:E:31:ILE:CG2	1:E:33:ARG:HG3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:VAL:H	1:F:204:ASN:ND2	2.05	0.54
1:D:19:ALA:HB2	1:D:39:VAL:HG12	1.90	0.54
1:B:289:HIS:C	1:B:291:ILE:N	2.64	0.54
1:E:258:ASN:ND2	1:E:259:GLU:H	2.06	0.54
1:F:13:GLU:O	1:F:14:LEU:O	2.26	0.54
1:A:244:GLU:HG2	1:A:276:PHE:CD1	2.43	0.54
1:B:304:LYS:NZ	1:B:304:LYS:HB3	2.23	0.54
1:D:225:ARG:CG	1:D:275:GLU:HG2	2.37	0.54
1:C:280:ILE:HG13	1:C:313:ILE:HD12	1.89	0.54
1:F:13:GLU:HA	4:F:2551:HOH:O	2.08	0.54
1:A:278:VAL:HG12	1:A:305:VAL:HG11	1.89	0.53
1:D:34:ASP:HB2	4:D:2734:HOH:O	2.07	0.53
1:D:44:GLU:HA	1:D:85:SER:O	2.08	0.53
1:C:211:THR:CG2	1:C:212:GLY:N	2.71	0.53
1:C:258:ASN:ND2	1:C:259:GLU:H	2.02	0.53
1:C:278:VAL:HG12	1:C:305:VAL:HG11	1.91	0.53
1:F:31:ILE:HG23	1:F:33:ARG:HG3	1.89	0.53
1:A:26:GLU:HG3	4:A:2784:HOH:O	2.08	0.53
1:C:306:GLU:HG3	4:C:2600:HOH:O	2.09	0.53
1:E:225:ARG:CG	1:E:275:GLU:HG2	2.38	0.53
1:B:279:ASP:OD2	1:B:279:ASP:N	2.38	0.52
1:D:43:MET:HE3	1:D:84:PHE:HD1	1.74	0.52
1:F:43:MET:HE1	1:F:96:VAL:HG11	1.91	0.52
1:C:290:SER:HB2	1:C:293:ARG:HD2	1.92	0.52
1:E:33:ARG:NH2	1:E:78:ASP:OD2	2.42	0.52
1:A:23:HIS:HE1	4:A:2538:HOH:O	1.93	0.52
1:C:55:GLY:HA3	1:C:183:GLN:NE2	2.24	0.52
1:C:225:ARG:HG3	1:C:275:GLU:HG2	1.91	0.52
1:F:244:GLU:HG2	1:F:276:PHE:CD1	2.45	0.52
1:B:50:MET:HE3	1:B:60:TYR:CD1	2.44	0.52
1:D:289:HIS:C	1:D:291:ILE:N	2.67	0.52
1:E:211:THR:CG2	1:E:212:GLY:N	2.71	0.52
1:A:289:HIS:C	1:A:291:ILE:N	2.61	0.52
1:E:211:THR:HG23	1:E:302:GLN:CD	2.35	0.51
1:A:70:ARG:CZ	4:A:2562:HOH:O	2.58	0.51
1:B:95:ASN:HB3	1:B:112:PHE:HA	1.92	0.51
1:B:175:TYR:N	1:B:175:TYR:CD1	2.78	0.51
1:C:25:PRO:HD2	1:C:26:GLU:H	1.75	0.51
1:A:30:ALA:HA	1:A:73:ARG:CZ	2.41	0.51
1:A:280:ILE:HD12	1:A:313:ILE:HB	1.91	0.51
1:A:33:ARG:NH2	1:A:78:ASP:OD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:GLU:HA	4:D:2747:HOH:O	2.10	0.51
1:E:34:ASP:HB2	4:E:2711:HOH:O	2.11	0.51
1:D:264:THR:CG2	1:F:252:GLU:OE1	2.59	0.51
1:E:142:MET:HE2	1:E:188:PHE:HE2	1.76	0.51
1:F:43:MET:HE3	1:F:84:PHE:CD1	2.46	0.51
1:E:43:MET:HE2	1:E:82:VAL:CG1	2.41	0.50
1:E:226:MET:HE2	1:E:276:PHE:CE2	2.37	0.50
1:A:127:GLN:HE21	1:B:260:ASN:ND2	2.08	0.50
1:D:144:ILE:N	1:D:144:ILE:HD12	2.27	0.50
1:E:95:ASN:HB3	1:E:112:PHE:HA	1.92	0.50
1:D:127:GLN:HE21	1:E:260:ASN:ND2	2.07	0.50
1:D:286:LEU:HD23	1:D:286:LEU:N	2.27	0.50
1:F:289:HIS:C	1:F:291:ILE:N	2.67	0.50
1:A:258:ASN:ND2	1:A:259:GLU:H	2.08	0.50
1:B:173:ASP:OD1	1:B:233:PRO:HD2	2.11	0.50
1:B:33:ARG:N	4:B:594:HOH:O	2.45	0.49
1:B:112:PHE:O	1:B:117:ARG:NH1	2.45	0.49
1:F:87:ASN:ND2	1:F:89:SER:H	2.08	0.49
1:D:21:THR:OG1	1:D:70:ARG:HD3	2.12	0.49
1:A:112:PHE:O	1:A:117:ARG:NH1	2.45	0.49
1:A:264:THR:CG2	1:C:252:GLU:OE1	2.60	0.49
1:E:54:ASP:HB2	4:E:2734:HOH:O	2.11	0.49
1:F:281:PRO:HG2	1:F:307:GLY:C	2.37	0.49
1:E:33:ARG:HH22	1:E:78:ASP:CG	2.20	0.49
1:C:278:VAL:HG12	1:C:278:VAL:O	2.11	0.49
1:A:258:ASN:HD22	1:A:259:GLU:N	2.10	0.49
1:C:13:GLU:N	4:C:2684:HOH:O	2.45	0.49
1:D:256:LEU:H	1:E:258:ASN:ND2	2.11	0.49
1:D:258:ASN:ND2	1:F:256:LEU:H	2.10	0.49
1:D:260:ASN:ND2	1:F:127:GLN:HE21	2.10	0.49
1:D:286:LEU:HD23	1:D:286:LEU:H	1.77	0.49
1:E:32:ASP:C	4:E:2585:HOH:O	2.55	0.49
1:A:278:VAL:HG11	1:A:305:VAL:HG11	1.94	0.49
1:D:258:ASN:HD22	1:D:259:GLU:N	2.06	0.49
1:E:43:MET:HE3	1:E:84:PHE:HD1	1.78	0.49
1:B:175:TYR:CD2	1:B:193:ALA:HA	2.48	0.49
1:B:211:THR:HG23	1:B:302:GLN:CD	2.38	0.49
1:A:258:ASN:ND2	1:C:256:LEU:H	2.11	0.48
1:A:291:ILE:HG21	1:C:141:GLY:HA2	1.95	0.48
1:B:170:VAL:H	1:B:204:ASN:ND2	2.10	0.48
1:D:92:VAL:HB	4:D:2852:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ILE:HD11	1:E:74:VAL:HA	1.95	0.48
1:A:280:ILE:HD11	1:A:310:ASN:O	2.12	0.48
1:D:291:ILE:HG21	1:F:141:GLY:HA2	1.94	0.48
1:E:158:GLU:CD	1:E:158:GLU:H	2.21	0.48
1:A:225:ARG:CG	1:A:275:GLU:HG2	2.39	0.48
1:C:180:LYS:HD2	4:C:2797:HOH:O	2.13	0.48
1:E:304:LYS:NZ	1:E:304:LYS:HB3	2.28	0.48
1:E:141:GLY:HA2	1:F:291:ILE:HG21	1.94	0.48
1:E:286:LEU:N	1:E:286:LEU:HD23	2.27	0.48
1:F:173:ASP:OD1	1:F:233:PRO:HD2	2.13	0.48
1:D:252:GLU:OE1	1:E:264:THR:CG2	2.55	0.48
1:D:211:THR:CG2	1:D:212:GLY:H	2.27	0.48
1:D:291:ILE:CG2	1:D:292:PHE:N	2.77	0.48
1:A:250:TYR:HB2	1:A:273:ILE:HB	1.96	0.48
1:E:87:ASN:ND2	1:E:89:SER:H	2.10	0.48
1:A:117:ARG:HG2	1:A:118:THR:H	1.76	0.48
1:C:95:ASN:HB3	1:C:112:PHE:HA	1.95	0.48
1:F:242:ILE:HD12	1:F:285:THR:CG2	2.44	0.48
1:A:242:ILE:HB	1:A:285:THR:HG23	1.96	0.48
1:F:13:GLU:CD	1:F:38:LYS:NZ	2.72	0.48
1:F:180:LYS:NZ	4:F:2600:HOH:O	2.47	0.47
1:F:211:THR:CG2	1:F:212:GLY:N	2.77	0.47
1:B:127:GLN:HE21	1:C:260:ASN:ND2	2.11	0.47
1:E:127:GLN:HE21	1:F:260:ASN:ND2	2.12	0.47
1:A:170:VAL:H	1:A:204:ASN:ND2	2.12	0.47
1:F:31:ILE:HG22	1:F:33:ARG:HG3	1.95	0.47
1:F:292:PHE:O	1:F:296:ASN:HB2	2.14	0.47
1:B:211:THR:HG23	1:B:302:GLN:OE1	2.14	0.47
1:C:17:ILE:HD11	4:C:2558:HOH:O	2.14	0.47
1:D:314:MET:HG3	1:F:102:THR:O	2.14	0.47
1:A:256:LEU:HD21	1:B:256:LEU:HG	1.97	0.47
1:A:289:HIS:C	1:A:291:ILE:H	2.22	0.47
1:B:44:GLU:HA	1:B:85:SER:O	2.14	0.47
1:D:225:ARG:NH1	1:D:275:GLU:OE2	2.48	0.47
1:D:256:LEU:HB2	1:E:258:ASN:ND2	2.30	0.47
1:B:289:HIS:C	1:B:291:ILE:H	2.23	0.47
1:D:211:THR:HG23	1:D:302:GLN:OE1	2.15	0.47
1:A:25:PRO:HD2	1:A:26:GLU:H	1.80	0.47
1:C:310:ASN:OD1	1:C:312:GLU:HB2	2.14	0.47
1:D:70:ARG:NE	4:D:2603:HOH:O	2.46	0.47
1:E:190:MET:HG3	4:E:2720:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:MET:HE3	1:B:84:PHE:HD1	1.80	0.46
1:D:33:ARG:NH2	1:D:78:ASP:OD2	2.48	0.46
1:D:70:ARG:NH2	4:D:2603:HOH:O	2.47	0.46
1:E:261:VAL:HG11	1:E:264:THR:HG23	1.97	0.46
1:F:204:ASN:OD1	1:F:210:LEU:HD21	2.15	0.46
1:B:117:ARG:HG3	4:B:693:HOH:O	2.15	0.46
1:D:162:LYS:HE2	1:D:162:LYS:HA	1.96	0.46
1:C:242:ILE:HD12	1:C:285:THR:HG23	1.96	0.46
1:E:31:ILE:HG23	1:E:33:ARG:HG3	1.97	0.46
1:C:280:ILE:HD11	1:C:310:ASN:HB3	1.97	0.46
1:E:211:THR:HG23	1:E:302:GLN:OE1	2.15	0.46
1:D:256:LEU:H	1:E:258:ASN:HD21	1.63	0.46
1:E:117:ARG:HG3	4:E:2792:HOH:O	2.15	0.46
1:A:21:THR:OG1	1:A:70:ARG:HD3	2.16	0.46
1:B:250:TYR:HB2	1:B:273:ILE:HB	1.97	0.46
1:B:31:ILE:CG2	1:B:33:ARG:HG3	2.46	0.46
1:C:289:HIS:O	1:C:291:ILE:N	2.45	0.46
1:E:217:LYS:HE2	1:E:304:LYS:HD3	1.96	0.46
1:F:277:LYS:HE2	1:F:279:ASP:HB3	1.97	0.46
1:F:278:VAL:HG11	1:F:305:VAL:HG11	1.96	0.46
1:A:225:ARG:NH1	1:A:275:GLU:OE2	2.49	0.46
1:B:32:ASP:C	4:B:594:HOH:O	2.59	0.46
1:A:313:ILE:O	1:C:123:PHE:HA	2.16	0.45
1:D:33:ARG:HH22	1:D:78:ASP:CG	2.25	0.45
1:E:51:LYS:HE3	1:E:54:ASP:HA	1.98	0.45
1:F:44:GLU:HA	1:F:85:SER:O	2.16	0.45
1:E:23:HIS:CE1	4:E:2567:HOH:O	2.69	0.45
1:D:129:GLY:HA2	4:D:2659:HOH:O	2.16	0.45
1:E:44:GLU:HA	1:E:85:SER:O	2.17	0.45
1:E:258:ASN:HD22	1:E:259:GLU:N	2.13	0.45
1:F:286:LEU:N	1:F:286:LEU:HD23	2.32	0.45
1:B:51:LYS:HE2	1:B:54:ASP:HA	1.98	0.45
1:B:219:LYS:O	1:B:222:GLU:HG3	2.16	0.45
1:C:249:VAL:HG11	1:C:264:THR:CG2	2.39	0.45
1:A:211:THR:CG2	1:A:212:GLY:H	2.30	0.45
1:A:226:MET:HE1	1:A:241:VAL:HG21	1.98	0.45
1:B:165:LYS:HD2	1:B:222:GLU:OE2	2.16	0.45
1:C:31:ILE:HG23	1:C:33:ARG:HG3	1.97	0.45
1:A:277:LYS:HE2	1:A:279:ASP:HB3	1.98	0.45
1:A:292:PHE:O	1:A:296:ASN:HB2	2.17	0.44
1:F:14:LEU:N	4:F:2551:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:MET:HE1	1:F:241:VAL:HG21	1.98	0.44
1:B:43:MET:HE2	1:B:82:VAL:HG11	1.98	0.44
1:B:175:TYR:CE2	1:B:193:ALA:HA	2.51	0.44
1:A:281:PRO:HG2	1:A:307:GLY:C	2.42	0.44
1:B:225:ARG:HG3	1:B:225:ARG:HH11	1.82	0.44
1:C:31:ILE:HG23	1:C:33:ARG:CG	2.48	0.44
1:D:292:PHE:O	1:D:296:ASN:HB2	2.16	0.44
1:E:19:ALA:HB2	1:E:39:VAL:HG12	1.98	0.44
1:E:250:TYR:HB2	1:E:273:ILE:HB	2.00	0.44
1:F:289:HIS:C	1:F:291:ILE:H	2.25	0.44
1:C:142:MET:HE2	1:C:188:PHE:CD2	2.53	0.44
1:A:278:VAL:CG1	1:A:305:VAL:HG21	2.36	0.44
1:D:43:MET:HE1	1:D:96:VAL:HG11	2.00	0.44
1:D:211:THR:HG21	4:D:2814:HOH:O	2.18	0.44
1:F:281:PRO:CG	1:F:307:GLY:C	2.91	0.44
1:F:95:ASN:HB3	1:F:112:PHE:HA	2.00	0.44
1:D:210:LEU:HD22	1:D:216:LEU:HD21	2.00	0.44
1:A:70:ARG:NE	4:A:2562:HOH:O	2.50	0.44
1:E:170:VAL:H	1:E:204:ASN:ND2	2.16	0.44
1:F:51:LYS:HE3	1:F:54:ASP:HA	2.00	0.44
1:C:304:LYS:NZ	1:C:304:LYS:HB3	2.32	0.43
1:D:43:MET:HE3	1:D:84:PHE:CD1	2.53	0.43
1:D:97:ASP:OD2	1:D:97:ASP:C	2.61	0.43
1:D:310:ASN:OD1	1:D:312:GLU:HB2	2.18	0.43
1:A:280:ILE:HA	1:A:281:PRO:HD3	1.89	0.43
1:D:291:ILE:HG22	1:D:292:PHE:N	2.32	0.43
1:E:249:VAL:CG1	1:E:264:THR:HG21	2.30	0.43
1:C:250:TYR:HB2	1:C:273:ILE:HB	2.00	0.43
1:F:179:LYS:HE2	4:F:2765:HOH:O	2.18	0.43
1:D:175:TYR:N	1:D:175:TYR:CD1	2.86	0.43
1:E:175:TYR:N	1:E:175:TYR:CD1	2.86	0.43
1:F:236:VAL:CG1	1:F:265:ILE:HG23	2.48	0.43
1:A:186:GLN:HA	1:A:187:PRO:HD3	1.87	0.43
1:B:142:MET:HE2	1:B:188:PHE:CD2	2.53	0.43
1:C:170:VAL:H	1:C:204:ASN:HD21	1.67	0.43
1:C:180:LYS:HG2	1:C:200:TYR:CE2	2.53	0.43
1:E:16:VAL:HG11	1:E:40:ARG:NE	2.34	0.43
1:A:211:THR:HG23	1:A:302:GLN:OE1	2.19	0.43
1:C:50:MET:HE3	1:C:60:TYR:CD1	2.54	0.43
1:F:33:ARG:HH22	1:F:78:ASP:CG	2.27	0.43
1:F:142:MET:HE3	1:F:190:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:MET:CE	1:F:276:PHE:HE2	2.23	0.43
1:F:280:ILE:HA	1:F:281:PRO:HD3	1.89	0.43
1:D:162:LYS:HE3	4:D:2583:HOH:O	2.18	0.43
1:E:112:PHE:O	1:E:117:ARG:NH1	2.52	0.43
1:B:278:VAL:CG1	1:B:305:VAL:HG21	2.24	0.43
1:D:225:ARG:HG3	1:D:225:ARG:HH11	1.84	0.43
1:D:280:ILE:HA	1:D:281:PRO:HD3	1.89	0.43
1:A:310:ASN:OD1	1:A:312:GLU:HB2	2.19	0.42
1:B:43:MET:HE2	1:B:82:VAL:CG1	2.49	0.42
1:B:186:GLN:HA	1:B:187:PRO:HD3	1.90	0.42
1:A:291:ILE:HG22	1:A:292:PHE:N	2.35	0.42
1:C:211:THR:HG23	1:C:302:GLN:OE1	2.18	0.42
4:A:2529:HOH:O	1:B:297:LYS:HE3	2.20	0.42
1:B:280:ILE:HA	1:B:281:PRO:HD3	1.91	0.42
1:D:114:ALA:H	1:D:117:ARG:HD2	1.85	0.42
1:E:122:SER:O	1:F:314:MET:HA	2.19	0.42
1:F:142:MET:HE2	1:F:188:PHE:CD2	2.54	0.42
1:C:13:GLU:CB	4:C:2684:HOH:O	2.67	0.42
1:C:281:PRO:HG2	1:C:307:GLY:C	2.44	0.42
1:B:27:VAL:HG13	1:B:71:MET:SD	2.60	0.42
1:E:33:ARG:HD3	4:E:2795:HOH:O	2.19	0.42
1:E:175:TYR:CD2	1:E:193:ALA:HA	2.54	0.42
1:F:97:ASP:O	1:F:133:TYR:HA	2.20	0.42
1:A:36:PRO:HA	4:A:2568:HOH:O	2.20	0.42
1:B:87:ASN:HA	1:B:88:PRO:HD3	1.95	0.42
1:E:162:LYS:HA	1:E:162:LYS:CE	2.45	0.42
1:F:176:THR:CG2	1:F:186:GLN:HB3	2.40	0.42
1:A:55:GLY:HA3	1:A:183:GLN:HE22	1.84	0.42
1:B:252:GLU:OE1	1:C:264:THR:HG22	2.20	0.42
1:D:27:VAL:HG13	1:D:71:MET:CE	2.49	0.42
1:D:175:TYR:CD2	1:D:193:ALA:HA	2.55	0.42
1:E:31:ILE:CD1	1:E:74:VAL:C	2.92	0.42
1:F:217:LYS:HD3	1:F:304:LYS:HB2	2.01	0.42
1:A:142:MET:HG3	1:A:188:PHE:CE2	2.55	0.42
1:B:280:ILE:HD13	4:B:772:HOH:O	2.20	0.41
1:C:281:PRO:CG	1:C:307:GLY:C	2.93	0.41
1:E:142:MET:HE3	1:E:142:MET:HB2	1.84	0.41
1:B:97:ASP:OD2	1:B:97:ASP:C	2.63	0.41
1:B:210:LEU:HD22	1:B:216:LEU:HD21	2.03	0.41
1:C:280:ILE:HA	1:C:281:PRO:HD3	1.91	0.41
1:E:180:LYS:HD3	4:E:2601:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PRO:HD2	1:B:26:GLU:H	1.84	0.41
1:B:236:VAL:CG1	1:B:265:ILE:HG23	2.49	0.41
1:D:280:ILE:HD11	1:D:310:ASN:O	2.20	0.41
1:A:44:GLU:HA	1:A:85:SER:O	2.20	0.41
1:A:142:MET:HE2	1:A:188:PHE:CD2	2.55	0.41
1:E:225:ARG:NH1	1:E:275:GLU:OE2	2.52	0.41
1:B:81:GLU:CD	4:B:662:HOH:O	2.63	0.41
1:B:189:ASP:CG	4:B:540:HOH:O	2.63	0.41
1:D:144:ILE:N	1:D:144:ILE:CD1	2.84	0.41
1:D:304:LYS:HB3	1:D:304:LYS:NZ	2.35	0.41
1:A:35:TYR:HA	1:A:36:PRO:HD3	1.91	0.41
1:C:292:PHE:O	1:C:296:ASN:HB2	2.20	0.41
1:E:280:ILE:HD13	4:E:2743:HOH:O	2.19	0.41
1:D:226:MET:HE3	1:D:274:VAL:HG21	2.02	0.41
1:E:144:ILE:HD13	1:F:291:ILE:HD13	1.72	0.41
1:F:170:VAL:H	1:F:204:ASN:HD21	1.67	0.41
1:A:280:ILE:HD11	1:A:310:ASN:HB3	2.03	0.41
1:D:186:GLN:HA	1:D:187:PRO:HD3	1.91	0.41
1:A:142:MET:HG3	1:A:188:PHE:CD2	2.56	0.41
1:A:142:MET:HE2	1:A:188:PHE:CE2	2.56	0.41
1:B:170:VAL:H	1:B:204:ASN:HD21	1.68	0.41
1:C:279:ASP:OD2	1:C:279:ASP:N	2.41	0.41
1:D:242:ILE:HD12	1:D:285:THR:CG2	2.48	0.41
1:F:13:GLU:CD	1:F:38:LYS:HZ1	2.29	0.41
1:F:31:ILE:HG23	1:F:33:ARG:CG	2.50	0.41
1:F:55:GLY:HA3	1:F:183:GLN:HE22	1.86	0.41
1:C:175:TYR:CD1	1:C:175:TYR:N	2.90	0.41
1:D:256:LEU:HG	1:F:256:LEU:HD21	2.03	0.41
1:D:291:ILE:HD13	1:D:291:ILE:HA	1.86	0.41
1:F:68:PRO:HD3	1:F:204:ASN:HA	2.03	0.41
1:A:268:ALA:O	1:B:289:HIS:HB3	2.20	0.40
1:C:87:ASN:ND2	1:C:89:SER:H	2.12	0.40
1:D:226:MET:HE3	1:D:274:VAL:CG2	2.51	0.40
1:F:36:PRO:HA	4:F:2556:HOH:O	2.22	0.40
1:F:179:LYS:HA	1:F:199:GLU:CD	2.46	0.40
1:D:113:THR:HG23	1:D:117:ARG:HD2	2.03	0.40
1:A:260:ASN:HD22	1:C:127:GLN:HE21	1.69	0.40
1:D:101:ALA:HB1	1:E:314:MET:CE	2.51	0.40
1:D:173:ASP:OD1	1:D:233:PRO:HD2	2.21	0.40
1:D:279:ASP:OD2	1:D:279:ASP:N	2.51	0.40
1:E:219:LYS:O	1:E:222:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ARG:NH2	1:C:37:ALA:HB3	2.37	0.40
1:D:87:ASN:HA	1:D:88:PRO:HD3	1.95	0.40
1:E:43:MET:HE1	1:E:96:VAL:HG11	2.04	0.40
1:B:13:GLU:HG3	1:B:14:LEU:H	1.86	0.40
1:B:258:ASN:HD22	1:B:259:GLU:H	1.69	0.40
1:D:175:TYR:CE2	1:D:193:ALA:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/327 (92%)	290 (97%)	8 (3%)	2 (1%)	18	10
1	B	300/327 (92%)	289 (96%)	9 (3%)	2 (1%)	18	10
1	C	300/327 (92%)	288 (96%)	10 (3%)	2 (1%)	18	10
1	D	300/327 (92%)	289 (96%)	9 (3%)	2 (1%)	18	10
1	E	300/327 (92%)	291 (97%)	8 (3%)	1 (0%)	36	28
1	F	300/327 (92%)	287 (96%)	10 (3%)	3 (1%)	12	5
All	All	1800/1962 (92%)	1734 (96%)	54 (3%)	12 (1%)	18	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	PRO
1	B	25	PRO
1	C	25	PRO
1	F	14	LEU
1	F	25	PRO
1	A	291	ILE

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Mol	Chain	Res	Type
1	B	291	ILE
1	C	291	ILE
1	E	291	ILE
1	F	291	ILE
1	D	291	ILE
1	D	205	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/259 (92%)	228 (95%)	11 (5%)	24	13
1	B	239/259 (92%)	227 (95%)	12 (5%)	22	11
1	C	239/259 (92%)	228 (95%)	11 (5%)	24	13
1	D	239/259 (92%)	225 (94%)	14 (6%)	18	7
1	E	239/259 (92%)	229 (96%)	10 (4%)	26	16
1	F	239/259 (92%)	228 (95%)	11 (5%)	24	13
All	All	1434/1554 (92%)	1365 (95%)	69 (5%)	23	12

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	46	VAL
1	A	121	PHE
1	A	158	GLU
1	A	173	ASP
1	A	176	THR
1	A	264	THR
1	A	280	ILE
1	A	285	THR
1	A	290	SER
1	A	291	ILE
1	B	33	ARG

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Mol	Chain	Res	Type
1	B	121	PHE
1	B	158	GLU
1	B	173	ASP
1	B	176	THR
1	B	180	LYS
1	B	264	THR
1	B	279	ASP
1	B	280	ILE
1	B	285	THR
1	B	286	LEU
1	B	291	ILE
1	C	33	ARG
1	C	121	PHE
1	C	158	GLU
1	C	173	ASP
1	C	176	THR
1	C	264	THR
1	C	279	ASP
1	C	280	ILE
1	C	285	THR
1	C	286	LEU
1	C	291	ILE
1	D	33	ARG
1	D	46	VAL
1	D	121	PHE
1	D	158	GLU
1	D	173	ASP
1	D	176	THR
1	D	225	ARG
1	D	264	THR
1	D	279	ASP
1	D	280	ILE
1	D	285	THR
1	D	286	LEU
1	D	291	ILE
1	D	314	MET
1	E	33	ARG
1	E	121	PHE
1	E	158	GLU
1	E	173	ASP
1	E	176	THR
1	E	264	THR

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Mol	Chain	Res	Type
1	E	280	ILE
1	E	285	THR
1	E	286	LEU
1	E	291	ILE
1	F	23	HIS
1	F	33	ARG
1	F	46	VAL
1	F	121	PHE
1	F	158	GLU
1	F	173	ASP
1	F	176	THR
1	F	264	THR
1	F	279	ASP
1	F	285	THR
1	F	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	87	ASN
1	A	183	GLN
1	A	197	GLN
1	A	204	ASN
1	A	258	ASN
1	B	87	ASN
1	B	183	GLN
1	B	204	ASN
1	B	258	ASN
1	B	260	ASN
1	C	87	ASN
1	C	127	GLN
1	C	183	GLN
1	C	204	ASN
1	C	258	ASN
1	C	260	ASN
1	D	23	HIS
1	D	87	ASN
1	D	183	GLN
1	D	197	GLN
1	D	204	ASN
1	D	258	ASN

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Mol	Chain	Res	Type
1	D	260	ASN
1	E	23	HIS
1	E	87	ASN
1	E	197	GLN
1	E	204	ASN
1	E	258	ASN
1	E	260	ASN
1	F	23	HIS
1	F	87	ASN
1	F	183	GLN
1	F	204	ASN
1	F	258	ASN
1	F	260	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NO2	E	2507	2	1,2,2	4.69	1 (100%)	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NO2	A	2504	2	1,2,2	4.64	1 (100%)	0,1,1	-	-
3	NO2	F	2508	2	1,2,2	4.63	1 (100%)	0,1,1	-	-
3	NO2	A	2506	2	1,2,2	4.59	1 (100%)	0,1,1	-	-
3	NO2	D	2509	2	1,2,2	4.65	1 (100%)	0,1,1	-	-
3	NO2	C	2505	2	1,2,2	4.61	1 (100%)	0,1,1	-	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2507	NO2	O1-N	4.69	1.45	1.22
3	D	2509	NO2	O1-N	4.65	1.45	1.22
3	A	2504	NO2	O1-N	4.64	1.45	1.22
3	F	2508	NO2	O1-N	4.63	1.45	1.22
3	C	2505	NO2	O1-N	4.61	1.45	1.22
3	A	2506	NO2	O1-N	4.59	1.45	1.22

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2507	NO2	1	0
3	A	2504	NO2	1	0
3	F	2508	NO2	1	0
3	A	2506	NO2	1	0
3	D	2509	NO2	1	0
3	C	2505	NO2	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	302/327 (92%)	0.28	26 (8%) 16 19	12, 20, 35, 59	0
1	B	302/327 (92%)	0.26	14 (4%) 37 43	12, 21, 33, 51	0
1	C	302/327 (92%)	0.43	26 (8%) 16 19	13, 23, 38, 55	0
1	D	302/327 (92%)	0.31	26 (8%) 16 19	12, 20, 36, 55	0
1	E	302/327 (92%)	0.40	19 (6%) 26 30	12, 23, 36, 49	0
1	F	302/327 (92%)	0.44	26 (8%) 16 19	13, 22, 37, 58	0
All	All	1812/1962 (92%)	0.35	137 (7%) 20 22	12, 22, 36, 59	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	ASP	5.7
1	F	308	ALA	5.6
1	F	13	GLU	5.6
1	D	314	MET	5.4
1	C	280	ILE	5.4
1	F	32	ASP	5.2
1	A	117	ARG	4.9
1	D	278	VAL	4.8
1	F	307	GLY	4.7
1	F	34	ASP	4.6
1	B	32	ASP	4.6
1	E	54	ASP	4.6
1	C	32	ASP	4.6
1	D	34	ASP	4.5
1	A	313	ILE	4.3
1	A	280	ILE	4.2
1	C	117	ARG	4.1
1	D	280	ILE	4.1
1	C	24	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	34	ASP	4.0
1	B	211	THR	4.0
1	A	278	VAL	4.0
1	F	117	ARG	3.9
1	B	309	GLU	3.9
1	D	211	THR	3.9
1	B	210	LEU	3.8
1	D	117	ARG	3.8
1	E	278	VAL	3.8
1	C	211	THR	3.7
1	E	211	THR	3.7
1	B	34	ASP	3.7
1	D	313	ILE	3.7
1	E	309	GLU	3.6
1	C	210	LEU	3.6
1	F	313	ILE	3.6
1	B	117	ARG	3.6
1	E	117	ARG	3.6
1	F	291	ILE	3.5
1	F	211	THR	3.4
1	A	308	ALA	3.4
1	D	210	LEU	3.4
1	D	309	GLU	3.3
1	B	278	VAL	3.3
1	C	314	MET	3.3
1	E	32	ASP	3.3
1	A	24	ALA	3.3
1	E	210	LEU	3.2
1	E	291	ILE	3.2
1	C	307	GLY	3.2
1	A	34	ASP	3.2
1	F	24	ALA	3.1
1	F	311	PRO	3.1
1	D	24	ALA	3.1
1	E	307	GLY	3.1
1	D	13	GLU	3.1
1	A	279	ASP	3.0
1	E	280	ILE	3.0
1	F	14	LEU	3.0
1	A	314	MET	3.0
1	A	304	LYS	3.0
1	A	54	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	211	THR	2.9
1	C	308	ALA	2.9
1	A	210	LEU	2.9
1	C	309	GLU	2.9
1	F	210	LEU	2.9
1	F	278	VAL	2.8
1	C	13	GLU	2.8
1	C	312	GLU	2.8
1	E	313	ILE	2.7
1	A	310	ASN	2.7
1	A	309	GLU	2.7
1	F	314	MET	2.7
1	A	33	ARG	2.7
1	D	307	GLY	2.7
1	A	163	VAL	2.7
1	D	308	ALA	2.6
1	A	306	GLU	2.6
1	C	291	ILE	2.6
1	D	306	GLU	2.6
1	D	279	ASP	2.6
1	F	280	ILE	2.6
1	F	310	ASN	2.5
1	E	163	VAL	2.5
1	D	311	PRO	2.5
1	B	24	ALA	2.5
1	E	308	ALA	2.5
1	E	36	PRO	2.5
1	D	32	ASP	2.5
1	A	307	GLY	2.4
1	D	33	ARG	2.4
1	A	13	GLU	2.4
1	C	311	PRO	2.4
1	A	32	ASP	2.4
1	C	313	ILE	2.4
1	A	311	PRO	2.4
1	C	279	ASP	2.3
1	E	13	GLU	2.3
1	B	280	ILE	2.3
1	D	291	ILE	2.3
1	F	179	LYS	2.3
1	D	223	THR	2.3
1	C	281	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	163	VAL	2.3
1	F	81	GLU	2.3
1	E	14	LEU	2.3
1	D	176	THR	2.3
1	F	223	THR	2.3
1	C	25	PRO	2.3
1	B	54	ASP	2.3
1	C	278	VAL	2.3
1	A	162	LYS	2.3
1	C	31	ILE	2.2
1	E	279	ASP	2.2
1	D	285	THR	2.2
1	F	279	ASP	2.2
1	C	157	LYS	2.2
1	F	26	GLU	2.2
1	C	223	THR	2.1
1	C	179	LYS	2.1
1	D	162	LYS	2.1
1	C	26	GLU	2.1
1	B	59	ARG	2.1
1	F	309	GLU	2.1
1	C	15	PRO	2.1
1	F	15	PRO	2.1
1	A	291	ILE	2.1
1	B	306	GLU	2.1
1	A	51	LYS	2.0
1	B	179	LYS	2.0
1	D	304	LYS	2.0
1	E	121	PHE	2.0
1	A	223	THR	2.0
1	B	15	PRO	2.0
1	D	157	LYS	2.0
1	F	162	LYS	2.0
1	F	163	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NO2	A	2506	3/3	0.90	0.14	27,27,32,33	0
3	NO2	A	2504	3/3	0.91	0.14	32,32,33,35	0
3	NO2	D	2509	3/3	0.92	0.14	26,26,29,32	0
3	NO2	E	2507	3/3	0.93	0.17	30,30,33,35	0
3	NO2	F	2508	3/3	0.94	0.15	31,31,34,35	0
3	NO2	C	2505	3/3	0.95	0.14	32,32,35,35	0
2	CU	D	501	1/1	0.99	0.02	20,20,20,20	0
2	CU	E	501	1/1	0.99	0.04	25,25,25,25	0
2	CU	A	501	1/1	0.99	0.02	20,20,20,20	0
2	CU	B	501	1/1	0.99	0.03	22,22,22,22	0
2	CU	F	501	1/1	1.00	0.02	22,22,22,22	0
2	CU	F	502	1/1	1.00	0.01	24,24,24,24	0
2	CU	C	501	1/1	1.00	0.02	21,21,21,21	0
2	CU	C	502	1/1	1.00	0.02	23,23,23,23	0
2	CU	A	502	1/1	1.00	0.02	21,21,21,21	0
2	CU	D	502	1/1	1.00	0.02	23,23,23,23	0
2	CU	B	502	1/1	1.00	0.02	24,24,24,24	0
2	CU	E	502	1/1	1.00	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.